Onset of $T=0$ Pairing and Deformations in High Spin States of the $N=Z$ Nucleus ^{48}Cr

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February 9, 2008

Abstract

The yrast line of the N=Z nucleus ^{48}Cr is studied up to high spins by means of the cranked Hartree-Fock-Bogoliubov method including the $T=0$ and $T=1$ isospin pairing channels. A Skyrme force is used in the mean-field channel together with a zero-range density-dependent interaction in the pairing channels. The extensions of the method needed to incorporate the neutron-proton pairing are summarized. The $T=0$ pairing correlations are found to play a decisive role for deformation properties and excitation energies above $16\hbar$ which is the maximum spin that can be obtained in the f7/2 subshell.

Pairing correlations play a crucial role in nuclear structure theory. They manifest themselves by the presence of a superfluid condensate in the ground state of even-even nuclei, which is responsible for the odd-even staggering of many nuclear properties. In most nuclei, pairs are formed by identical particles (protons or neutrons) moving in time-reversed orbits[1]. However, one expects neutron-proton (np) pairing correlations to become important close to the $N = Z$ line, since then protons and neutrons occupy the same shell model orbits[2].

Pairs formed by a neutron and a proton can be characterized by an isospin quantum number T equal either to 1 (as for pairing between identical nucleons) or 0. The properties of $T=0$ correlations are by far not as well understood as the $T=1$ correlations. In particular, not much is known about collective effects generated by the formation of $T=0$ pairs.

Early studies of np correlations were mainly limited to light mass nuclei and schematic forces[2, 3, 4, 5]. The interest in np pairing correlations has been renewed[6, 7] by the experimental possibilities opened by the event of powerful detector arrays. It is indeed now possible to

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extend our knowledge on the structure of $N = Z$ nuclei to medium mass nuclei. In this paper, we will study the nucleus ^{48}Cr that has been investigated at Chalk River [8] and Legnaro [9] up to high angular momenta.

The strongest evidence for np pairing comes up to now from masses. It has been shown[10] that the systematics of the nuclear masses for constant nucleon number A presents a cusp at $N=Z$ and that this feature may be at least partly attributed to the np pairing[12, 7]. The $T=0$ pairs should also manifest themselves in the structure of excited states. The properties of rotational bands which have been an important tool to study the effects of particle-like pairing may also be appropriate for the study of np pairing. Cranked mean-field and Monte-Carlo shell-model calculations [3, 4, 7, 11] have shown that the $T=0$ pairing field is more resistant against nuclear rotation than the $T=1$ pairing. High spin states of $N=Z$ nuclei may therefore be sensitive to the properties of $T=0$ pairing.

In this letter, we present a study of the structure of high angular momentum states of ^{48}Cr. We have developed a cranked Hartree-Fock-Bogoliubov (CHFB) method with a Skyrme force in the mean-field channel and density-dependent zero-range pairing forces for the $T=0$ and $T=1$ pairing channels. This is the first time that a Skyrme force is used in a calculation including the $T=0$ pairing channel.

The yrast line of ^{48}Cr is known experimentally [8, 9] up to an angular momentum I of $16\hbar$. It reveals a backbend in a plot of spin as a function of rotational frequency at a spin around $12\hbar$. This backbend is related to a change from collective to non-collective states induced by the alignment of the f$_{7/2}$ orbits[15]. The highest observed state has a spin of $16\hbar$ which exhausts the f$_{7/2}$ shell. A previous CHFB calculation[15] has shown that the ground state of ^{48}Cr is prolate and that the shape evolves along the yrast line up to sphericity at a spin of $16\hbar$. ^{48}Cr has also been studied by the shell model[15, 16]. Both shell model and CHF calculations reproduce successfully the backbending of the yrast line, although the CHF backbending curve is too low in angular velocity when compared to experiment. States with $I > 16\hbar$ have not been determined in these works. The full fp shell has been included in the shell model space, but states with spins higher than $20\hbar$ need an extension of the space to the sd-shell and the g$_{9/2}$ subshell. Such calculations are beyond present shell-model techniques.

Since the mean field method describes rather successfully the low spin spectrum of ^{48}Cr without introducing $T=0$ correlations, we shall focus in this paper on the states beyond the 'terminating' point at $I=16\hbar$. Our main aim is to determine to what extent the $T=0$ correlations will affect their structure.

A new method of solution of the cranked Skyrme-HFB equations has been presented in recent publications[17, 18]. It combines the imaginary-time evolution method to determine the basis which diagonalizes the mean-field hamiltonian and a diagonalization of the HFB hamiltonian matrix calculated in the HF basis to construct the canonical basis. Different interactions are used in the mean-field and pairing channels: a Skyrme force for the mean-field and either a seniority[17] or a zero-range density-dependent interaction[18] for the pairing field. The pairing correlations were limited to like particle interactions. One of the important features of this method is a separation of the mean-field and pairing field equations, with however full self-consistency between them.

To allow a simultaneous treatment of all forms of pairing, one has to generalize the Bogoli-

ubov transformation. As a consequence, the mean-field equations have to be modified: when pairing is limited to like particles, pairs are formed by states of opposite signatures. Since np pairs can occupy identical states, the signature is lost as a good quantum number by the general Bogoliubov transformation[4, 19]. Let c_i^n and c_i^p be respectively the neutron and proton annihilation operators in the states i diagonalizing the HF equations, with $\mathcal{M}_n$ neutron and $\mathcal{M}_p$ proton basis states. The Bogoliubov transformation from this single-particle basis to the quasiparticle basis in which the CHFB Hamiltonian is diagonal can be written as

$$
\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} \overline{U}_n{}^\dagger & \overline{U}_p{}^\dagger & \overline{V}_n{}^\dagger & \overline{V}_p{}^\dagger \\ \overline{V}_n{}^T & \overline{V}_p{}^T & \overline{U}_n{}^T & \overline{U}_p{}^T \end{pmatrix} \begin{pmatrix} c^n \\ c^p \\ c^{n\dagger} \\ c^{p\dagger} \end{pmatrix},
\tag{1}
$$

where a stands for an annihilation operator of a quasiparticle state, $\overline{U}_n{}^\dagger$ ($\overline{V}_n{}^\dagger$) are block matrices, and T denotes the transposition of a matrix. Note that the number of the quasiparticle operators $\{a\}$ is $\mathcal{M}_n + \mathcal{M}_p$, and the size of $\overline{U}_n{}^\dagger$ and $\overline{V}_n{}^\dagger$ is $(\mathcal{M}_n + \mathcal{M}_p) \times \mathcal{M}_n$. $\overline{U}_p{}^\dagger$ and $\overline{V}_p{}^\dagger$ are $(\mathcal{M}_n + \mathcal{M}_p) \times \mathcal{M}_p$ matrices. The quasiparticle states are now mixing protons and neutrons.

It has been shown that when parity and signature are good quantum numbers and with an appropriate choice of phase, the HF wave functions can be represented in the $x, y, z \geq 0$ octant of a box in $\mathbf{r}$-space [20]. The complete description of the single particle wave functions requires then four real functions corresponding to the real and imaginary parts of the spin-up and spin-down components. The signature symmetry being lost, the space to be considered can only be reduced to a quarter of a box.

The method introduced in ref [18] can be rather easily extended to this new case. After diagonalization of the Bogoliubov equations written in the HF basis, the density matrix can be constructed and diagonalized. The wave-functions in the canonical basis have now 8 components since proton and neutron states are mixed by the pairing correlations. The density is given by:

$$
\rho(\mathbf{r}) = \sum_{i,\sigma\tau} v_i^2 |\varphi_i(\mathbf{r}, \sigma, \tau)|^2
\tag{2}
$$

where $\varphi_i(\mathbf{r}, \sigma, \tau)$ is the complex (σ, τ) component of the ith canonical basis wave-function; σ and τ denote the spin and isospin respectively and v_i^2 is an eigenvalue of the density matrix.

Parlińska et al. [21] have derived the new terms that arise in a Skyrme force when the densities mix protons and neutrons. For simplicity, and since we use different interactions in the mean-field and pairing channels, we have not introduced these terms. Densities for protons and neutrons are defined by limiting the summations in equ. (2) to τ equal either to $1/2$ or $-1/2$. The occupations of neutron and proton states is then given by $\int d^3\mathbf{r} \sum_{i,\sigma} v_i^2 |\varphi_i(\mathbf{r}, \sigma, \tau)|^2$.

In the following, we have used the parameter set SIII for the Skyrme interaction[22] and a zero-range pairing force as in ref.[18]:

$$
V_T(\mathbf{r_1}, \mathbf{r_2}) = G_T(1 - \rho(\mathbf{r_1})/\rho_c)\, \delta(\mathbf{r_1} - \mathbf{r_2}),
\tag{3}
$$

where G_T is the strength of the interaction and ρ_c a constant taken equal to 0.16 fm^{-3}, a value close to the nuclear saturation density. In this way, $V_T(\mathbf{r_1}, \mathbf{r_2})$ is peaked at the surface

of the nucleus. Assuming isospin invariance, the same strength has been used for all the $T=1$ components of the pairing force. We have fixed $G_{T=1}$ to 1000 MeV fm^3, which is the value used in a previous HFB calculation of the ground state properties of Mg isotopes far from stability[23]. As usual, a smooth cut-off of the pairing force has been introduced 5 MeV above the energy of the Fermi level. For the strength of the $T=0$ correlations, we have chosen to scale the $T=1$ strength by a factor equal to 1.3. This choice originates from proton-neutron scattering data that show clearly the spin singlet ($S=0$) interaction to be weaker than the triplet ($S=1$) one, resulting in a ratio of ≈ 1.3 for $G_{T=0}/G_{T=1}$ [24].

Using the antisymmetry of the pairing tensor κ and with a calculation similar to that of ref[18], one can write the pairing field Δ in a way suitable for computation and decompose it into its $T=1$ and 0 components:

$$
\begin{aligned}
\Delta_{(i\tau)(j\,\tau')} &= \int d^3\mathbf{r} \sum_{\sigma\sigma'} \phi_i^*(\mathbf{r},\sigma,\tau)\,\phi_j^*(\mathbf{r},\sigma',\tau') \\
&\times \left\{ \delta_{\tau,-\tau'}(-)^{\frac{1}{2}-\tau}\sqrt{2}^{-1+|\sigma+\sigma'|}\Delta_{T=0,S_z=\sigma+\sigma'}(\mathbf{r}) \right. \\
&\left. + \delta_{\sigma,-\sigma'}(-)^{\frac{1}{2}-\sigma}\sqrt{2}^{-1+|\tau+\tau'|}\Delta_{T=1,T_z=\tau+\tau'}(\mathbf{r}) \right\} ,
\end{aligned}
\tag{4}
$$

$$
\Delta_{T=0,S_z}(\mathbf{r}) = -v_{T=0}(\mathbf{r})\sum_{kl}\sum_{\sigma\sigma'}\langle\tfrac{1}{2}\sigma\tfrac{1}{2}\sigma'|1S_z\rangle\phi_k(\mathbf{r},\sigma,\tfrac{1}{2})\phi_l(\mathbf{r},\sigma',-\tfrac{1}{2})\kappa_{(k\frac{1}{2})(l-\frac{1}{2})} ,
\tag{5}
$$

$$
\Delta_{T=1,T_z}(\mathbf{r}) = -v_{T=1}(\mathbf{r})\sum_{kl}\sum_{\tau\tau'}\langle\tfrac{1}{2}\tau\tfrac{1}{2}\tau'|1T_z\rangle\phi_k(\mathbf{r},\tfrac{1}{2},\tau)\phi_l(\mathbf{r},-\tfrac{1}{2},\tau')\kappa_{(k\tau)(l\tau')} ,
\tag{6}
$$

$$
v_{T=1,0}(\mathbf{r}) = G_{T=1,0}\left(1 - \rho(\mathbf{r})/\rho_c\right) ,
\tag{7}
$$

where $\phi_i(\mathbf{r},\sigma,\tau)$ is the ith single-particle wave function in the HF basis.

The spin singlet $S=0$ with $T_z=\pm1$ term in equ. (6) corresponds to the usual pairing interaction between signature-reversed states. The np pairing interaction appears in both the spin singlet ($T=1$) and the spin triplet ($T=0$) modes. Note the symmetry between the spin anti-symmetric (isospin symmetric) state ($S=0$, $T=1$) and spin symmetric (isospin antisymmetric) state ($S=1$, $T=0$).

With the symmetries imposed in previous works[2] on the single-particle wave-functions, a real pairing tensor κ does not allow the simultaneous presence of all the pairing modes. A complex κ is then generated by a complex Bogoliubov transformation. The situation is different when, as here, parity is the only symmetry and the sp wave-functions are complex. When the system is time-reversal invariant, one can easily show that $T=0$ and $T=1$ pairing may be present at the same time. Using the relation between time reversed states given in ref [20], one obtains a purely imaginary $\Delta_{T=0,S_z=0}(\mathbf{r})$:

$$
\begin{aligned}
&\mathrm{Im}\Delta_{T=0,S_z=0}(\mathbf{r}) \\
&= -\sqrt{2}v_{T=0}(\mathbf{r})\sum_{\tau}(-)^{\frac{1}{2}-\tau}\sum_{\sigma}\left\{\sum_{ij}\mathrm{Re}\phi_i(\mathbf{r},\sigma,\tau)\,\mathrm{Im}\phi_j(\mathbf{r},-\sigma,-\tau)\kappa_{(i\tau)(j\,-\tau)} \right. \\
&\left. + \sum_{i\bar{j}}\mathrm{Re}\phi_i(\mathbf{r},\sigma,\tau)\,\mathrm{Im}\phi_{\bar{j}}(\mathbf{r},-\sigma,-\tau)\kappa_{(i\tau)(\bar{j}\,-\tau)}\right\} ,
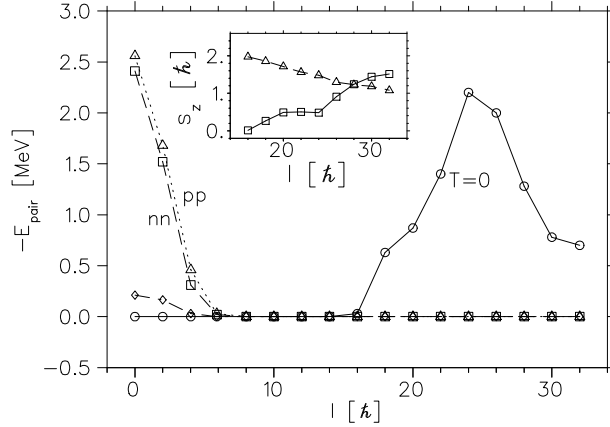\end{aligned}
\tag{8}
$$

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Figure 1: Pairing energies corresponding to the four pairing modes, along the yrast line. The energy of the $T=1$, $T_z = 0$ (np) component is represented by diamonds. The inset shows the expectation values of the total intrinsic spin along the rotational axis at high angular momenta. Squares and triangles correspond to positive and negative parity, respectively.

where $\overline{j}$ denotes a time-reversed state of j. In the same way, one can show that $\Delta_{T=1,S_z=0}(\mathbf{r})$ is real. Since the components of the pairing potential for all values of S_z and T_z may be present at the same time with a real pairing tensor, we have considered only real Bogoliubov transformations. In most of our results however, our solutions are dominated by either the $T=0$ or the $T=1$ pairing field. This difficulty of obtaining mixed solutions has been discussed in ref.[7] and is due to the lack of particle number and isospin conservations.

With a real pairing tensor, one can show that both the pairing and mean-field matrix elements are real, even when time reversal invariance is not assumed and signature is not a good quantum number. A detailed analysis of our method will be presented in a regular paper.

At low spins, we have found two solutions dominated by either the $T=1$ and $T=0$ pairing modes. Up to a spin of 16 $\hbar$, the two bands differ by their pairing properties but also by their deformation and excitation energies. For spins between 4 and 8 $\hbar$, the $T=0$ solution displays both pairing modes, illustrating the ability of our method to describe them simultaneously. We defer a detailed discussion of its properties to a forthcoming paper and limit our discussion of the low spin spectrum to the $T=1$ solution. The evolution of the four components of the pairing energy as a function of the angular momentum is plotted on Fig. 1. Pairing correlations disappear rapidly and for angular momenta between 6 and 16 $\hbar$, a pure CHF solution is obtained. At $16\hbar$, one reaches the total alignment of protons and neutrons in the $f_{7/2}$-shell. The higher spin states involve particle-hole excitations from the sd- and $f_{7/2}$-shells into the $g_{9/2}$- and $f_{5/2}$-shells. Above $I=16\hbar$, the $T=0$ pairing channel becomes active and persists up to the highest spins that we have studied. These $T=0$ correlations reach a maximum at $I = 24\hbar$.

The calculated spins as a function of frequency are compared to the experimental data on Fig. 2a. Up to $I = 16\hbar$, our results agree with previous CHFB calculations[15] using the
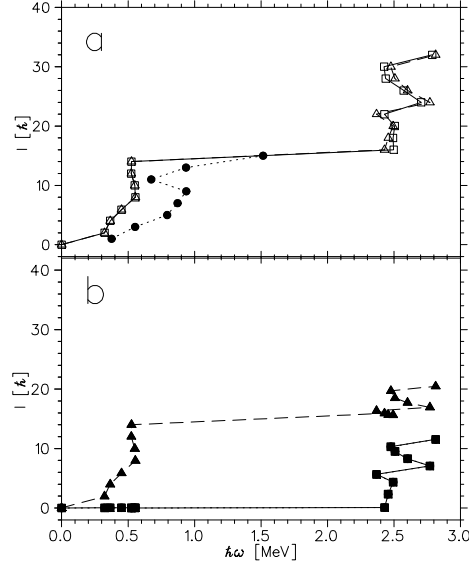
5

Figure 2: a)Variation of the angular momentum as a function of the rotational frequency along the yrast line. Our results are represented by □ for $G_{T=0} = 1.1G_{T=1}$ and △ for $G_{T=0} = 1.3G_{T=1}$ in the upper part. The experimental data (●) are taken from ref.[8, 9]. b)The contributions to the angular momentum coming from positive (squares) and negative parity states (triangles).
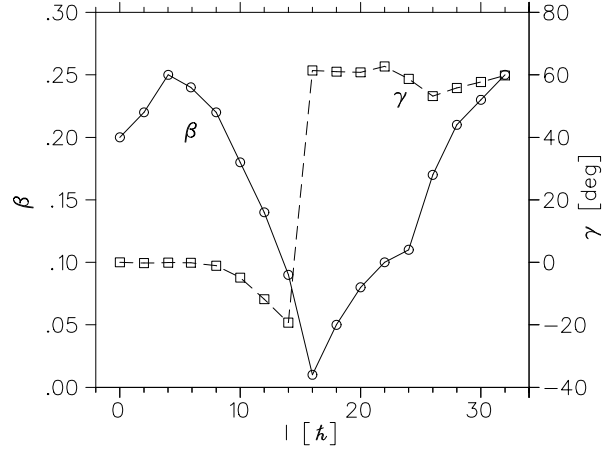

Figure 3: Variation of the quadrupole deformation (parameterized by β (circles) and γ (squares)) as a function of the rotational frequency along the yrast line.

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Gogny force. Like in those calculations, the spectrum is slightly too compressed with respect to the experimental data but the general agreement is satisfactory. Since pairing correlations are weak at low spin in ^{48}Cr, one can expect particle number projection techniques to decrease the moment of inertia at the bottom of the band and to improve the agreement with the data[15].

Above 16 $\hbar$, the structure of the yrast line changes. The γ transition energies become almost constant, around 5MeV, with two slight shifts at 24 and $32\hbar$. As illustrated on Fig. 2a, the results are not affected by decreasing the pairing strength from $G_{T=0} = 1.3G_{T=1}$ to $1.1G_{T=1}$. Note that solutions in the spin region $I = 18 - 30\hbar$ are obtained *only* in the presence of $T=0$ pairing correlations. If this mode is switched off, we have not been able to find neither CHFB nor pure CHF solutions; states can only be constructed as non collective multi-qp (or sp) states.

To generate spins above $16\hbar$, one can either promote particles from the $f_{7/2}$ subshell into the fp shell above the N(Z)=28 gap or via particle-hole excitations from $d_{3/2}$ into $g_{9/2}$. For both protons and neutrons, excitations into the $f_{5/2}$ yield a maximum gain in spin of $2\hbar$ while the $(d_{3/2})^{-1} - g_{9/2}$ ph excitations generate increases in spin up to $I=6\hbar$. At $I=0$, the energy of this $2\hbar\omega$ ph-excitation is of the order of 14 MeV but it is drastically reduced by rotation. For a cranking frequency around $2.5\hbar\omega$ MeV, the $d_{3/2}$ and $g_{9/2}$ levels are close to the Fermi surface.

The contributions of the different parities to the total spin are depicted in Fig. 2b. The main contributions above $16\hbar$ are coming from positive parity states. In our calculations, the occupation of the $g_{9/2}$ ($d_{3/2}$) grows (decreases) monotonically from 0(1) to 1(0.4) in the spin range of $16\hbar$ to $32\hbar$. It reaches 0.6(0.73) at $I = 24\hbar$ where the $T=0$ pairing energy has its maximum. However, np-pairs of negative parity contribute also to the $T=0$ correlations. At $32\hbar$, although pairing correlations are still sizable, the angular momentum is mainly generated by a few single particle levels: $(g_{9/2}\ d_{3/2}^{-1})_{6^+} \otimes (f_{7/2})^2_{6^+} \otimes (f_{7/2}\ f_{5/2})_{4^+}$ for both neutrons and protons.

The evolution of the quadrupole deformation calculated along the yrast line is shown on Fig.3. At low spin, ^{48}Cr is prolate; its deformation decreases above $I = 4\hbar$ and it becomes spherical at $I = 16\hbar$. Except for the small increase of deformation at low spin, our result is very similar to the one obtained with the Gogny force[15]. Above $I = 16\hbar$, the deformation is increasing smoothly with angular momentum. The nucleus is calculated to have an oblate shape rotating around the symmetry axis.

The deformation energy surface at $I = 24\hbar$ is shown on Fig. 4. It presents only an oblate minimum rather soft against deformation. [1] This may indicate that one should include dynamical fluctuations along the γ degree of freedom.

It is well established that deformation may be induced by the long range quadrupole-quadrupole force due to particle-hole excitations like $d_{3/2} - g_{9/2}$. The $T=0$ correlations induce a different and new type of collective excitations. The quadrupole deformation is now enhanced by the short-range $T=0$ np-force. The magnitude of the $T=0$ pairing correlations reflect the pair scattering from a np $d_{3/2}$ to a np $g_{9/2}$ pair. Since these pairs carry alignment, the smooth increase of their occupation result in an increase of the angular momentum which is of course correlated with the increase in deformation. Spin is also generated by the scattering of a np pair from the $f_{7/2}$ to the $f_{5/2}$ orbital. Both processes are only possible because the $T=0$ mode is

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[1]We also performed cranked Strutinsky type calculations, that show the existence of oblate super-deformed and prolate hyper-deformed solutions at $\approx$ 10MeV and $\approx$ 13MeV above the yrast $I=16\hbar$ state.
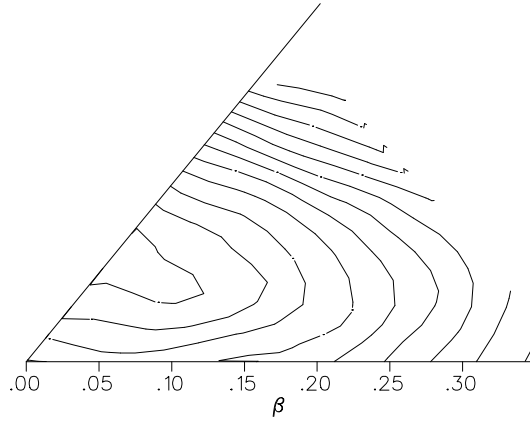
Figure 4: Potential energy surface calculated at $I = 24\hbar$. The minimum of the energy is obtained at $\beta = 0.11$, $\gamma = 60°$.

present. Thus, $T=0$ pairing correlations provide a new mechanism to generate angular momentum and quadrupole deformation beyond 'terminating states'. Note also that the $T=0$ pairing correlations become active in a spin regime, where one does not expect pairing to play any role.

The expectation value of the total intrinsic spin $< S_z >$ gives additional informations on the structure of the np pairs. Since the $d_{3/2}$ pair has its intrinsic spin $< s_z >$ coupled anti-parallel to the orbital angular momentum, the scattering into $g_{9/2}$ results in an increase of $< S_z >$. The opposite holds for the scattering from $f_{7/2}$ into $f_{5/2}$. The increase (decrease) in $< S_z >$ for the positive (negative) parity is shown in the inset of Fig. 1. Interestingly, in algebraic models, the main building blocks for neutron-proton pairing[25] are constructed by the coupling of a pair of spin orbit partners, like $f_{5/2}$ and $f_{7/2}$ to $L = 0$ and $S = J = 1$. In general, this coupling scheme is quenched above A=40 because the spin-orbit splitting becomes too large. We suggest that the reduction in the Wigner energy when going from the sd-shell to the fp-shell noticed by Satuła et al.[13], may be traced to this effect. We find here that such spin-orbit pairs may still play a role at high angular momenta.

A pure HF state can be constructed at $I=32\hbar$. Its deformation properties are compared to the CHFB solution in Table 1. Although pairing correlations are weak at $I=32\hbar$, the spreading in occupation probabilities that they generate results in a quadrupole moment much larger than that of the CHF state. On the other hand, the g-factor of the two solutions is quite close, around 0.52. In fact, the g-factor is nearly constant all along the yrast line and close to the value obtained with a Gogny force [15].

In summary, we have studied the properties of the high angular momentum states of ^{48}Cr, beyond the 'band termination' by means of the CHFB theory with both the $T=0$ and $T=1$ pairing channels taken into account. The only symmetry imposed on the wave-functions permit to limit oneselves to real Bogoliubov transformations and hence to have a real pairing tensor κ. We have shown that, contrary to previous studies where complex-HFB transformations had to be introduced, the two types of pairing interactions can be simultaneously present.

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		CHF	CHFB with T=0 pairing
Q_0	total [fm^2]	123	205
Q_c	charge [e fm^2]	63	104
β		0.16	0.26
γ	[deg]	60	59

Table 1: Total quadrupole moment (Q_0), charge quadrupole moment (Q_c) and deformation β and γ at I=32$\hbar$. γ=60° means oblate noncollective state.

The yrast line above 16$\hbar$ has properties intimately linked to the presence of T=0 pairing correlations: smooth increase of the quadrupole moment as a function of spin and nearly constant transition energies in the range 4.8 to 5.6 MeV. The T=0 correlations maximize exactly at half the maximum spin value of the involved configurations and induce a new type of collectivity. A spectacular effect of the np T=0 correlations is the presence of a much larger deformation at $I = 32\hbar$ than in the pure CHF state. All these properties should be fingerprints of the presence of T=0 pairing at high spins.

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